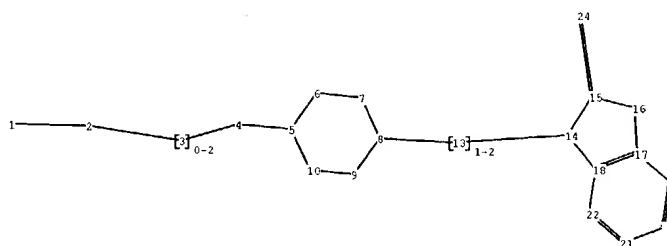
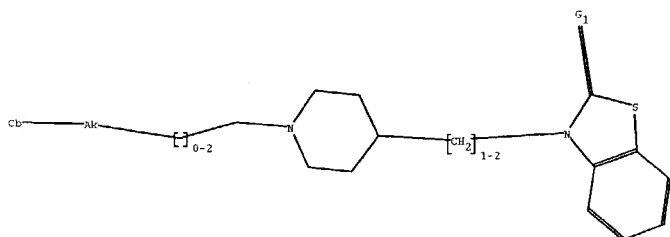


C:\stnweb\Queries\4.str



chain nodes :

1 2 3 4 13 24

ring nodes :

5 6 7 8 9 10 14 15 16 17 18 19 20 21 22

chain bonds :

1-2 2-3 3-4 4-5 8-13 13-14 15-24

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 14-15 14-18 15-16 16-17 17-18 17-19 18-22 19-20
20-21 21-22

exact/norm bonds :

1-2 2-3 4-5 5-6 5-10 6-7 7-8 8-9 9-10 14-15 14-18 15-24

exact bonds :

3-4 8-13 13-14 15-16 16-17

normalized bonds :

17-18 17-19 18-22 19-20 20-21 21-22

isolated ring systems :

containing 14 :

G1:O,S

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
24:CLASS

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 Jul 12 BEILSTEIN enhanced with new display and select options,
 resulting in a closer connection to BABS
NEWS 4 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display
 fields
NEWS 5 AUG 02 CAPLUS and CA patent records enhanced with European and Japan
 Patent Office Classifications
NEWS 6 AUG 02 The Analysis Edition of STN Express with Discover!
 (Version 7.01 for Windows) now available
NEWS 7 AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 8 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal
 status data from INPADOC
NEWS 9 SEP 01 INPADOC: New family current-awareness alert (SDI) available
NEWS 10 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
 STN Express with Discover!
NEWS 11 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 12 SEP 14 STN Patent Forum to be held October 13, 2004, in Iselin, NJ
NEWS 13 SEP 27 STANDARDS will no longer be available on STN
NEWS 14 SEP 27 SWETSCAN will no longer be available on STN

NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:41:29 ON 20 OCT 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	0.42

FILE 'REGISTRY' ENTERED AT 10:42:24 ON 20 OCT 2004

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STRUCTURE FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6
 DICTIONARY FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

=> s 11

SAMPLE SEARCH INITIATED 10:45:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 1 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 5 TO 234
 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 10:45:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 107 TO ITERATE

100.0% PROCESSED 107 ITERATIONS 26 ANSWERS
 SEARCH TIME: 00.00.01

L3 26 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	157.10	157.52

FILE 'HCAPLUS' ENTERED AT 10:45:15 ON 20 OCT 2004

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FILE COVERS 1907 - 20 Oct 2004 VOL 141 ISS 17
FILE LAST UPDATED: 19 Oct 2004 (20041019/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 1 L3

=> d 14, ibib abs fhitstr, 1

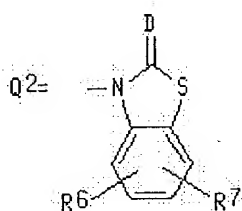
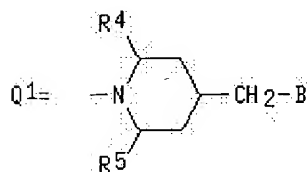
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text References

ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 9923083</u>	A1	19990514	<u>WO 1998-JP4973</u>	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
<u>EP 1043319</u>	A1	20001011	<u>EP 1998-951687</u>	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
<u>JP 11217377</u>	A2	19990810	<u>JP 1998-314459</u>	19981105
PRIORITY APPLN. INFO.:			<u>JP 1997-302607</u>	A 19971105
			<u>WO 1998-JP4973</u>	W 19981104

OTHER SOURCE(S): MARPAT 130:338102
GI



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxy-carbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ -receptors and exhibit small inhibition consts. K_i against σ -1 and/or σ -2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to σ -receptor (P2 membrane fraction) prepn. from rat liver with K_i value of 7.0 and 3.1 nM, resp., as compared to K_i of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

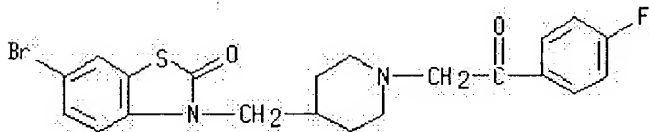
IT 224443-05-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



HCl

REFERENCE COUNT:

17

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> file caold
COST IN U.S. DOLLARS                SINCE FILE      TOTAL
                                     ENTRY      SESSION
FULL ESTIMATED COST                9.48        167.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                     ENTRY      SESSION
CA SUBSCRIBER PRICE                -0.70        -0.70
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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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=> d his

(FILE 'HOME' ENTERED AT 10:41:29 ON 20 OCT 2004)

FILE 'REGISTRY' ENTERED AT 10:42:24 ON 20 OCT 2004

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L1      STRUCTURE UPLOADED
L2      1 S L1
L3      26 S L1 FULL
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FILE 'HCAPLUS' ENTERED AT 10:45:15 ON 20 OCT 2004

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L4      1 S L3
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FILE 'CAOLD' ENTERED AT 10:46:26 ON 20 OCT 2004

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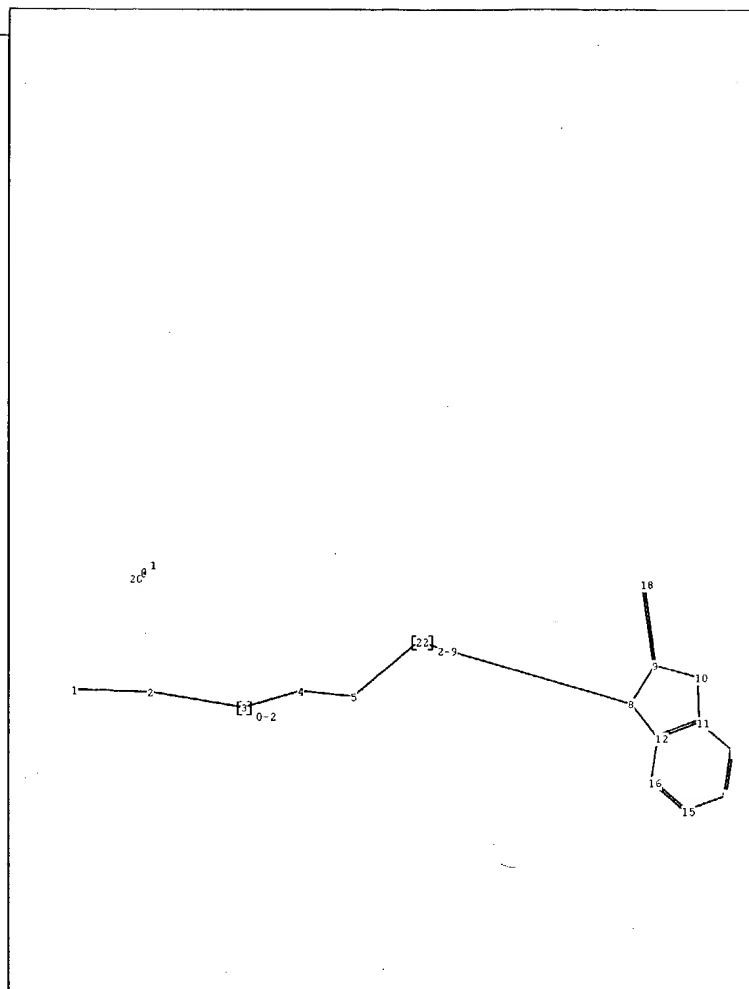
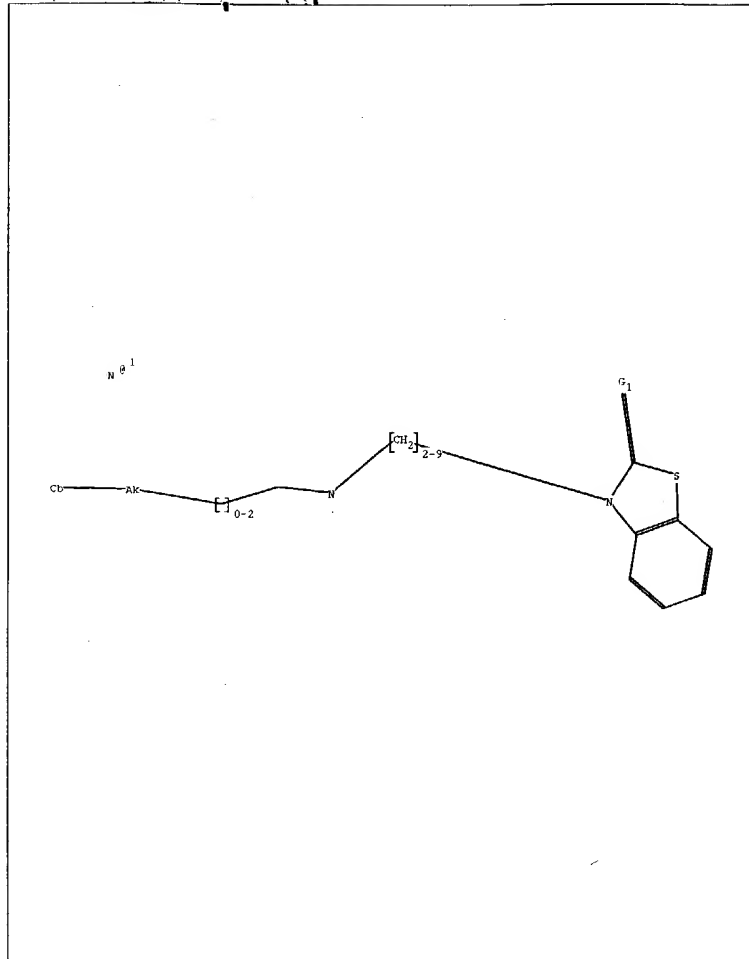
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                                     ENTRY      SESSION
FULL ESTIMATED COST                0.42        167.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                     ENTRY      SESSION
CA SUBSCRIBER PRICE                0.00        -0.70
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STN INTERNATIONAL LOGOFF AT 10:46:39 ON 20 OCT 2004



chain nodes :

1 2 3 4 5 18 20 22

ring nodes :

8 9 10 11 12 13 14 15 16

chain bonds :

1-2 2-3 3-4 4-5 5-22 8-22 9-18

ring bonds :

8-12 8-9 9-10 10-11 11-12 11-13 12-16 13-14 14-15 15-16

exact/norm bonds :

1-2 2-3 4-5 8-9 9-18

exact bonds :

3-4 5-22 8-12 8-22 9-10 10-11

normalized bonds :

11-12 11-13 12-16 13-14 14-15 15-16

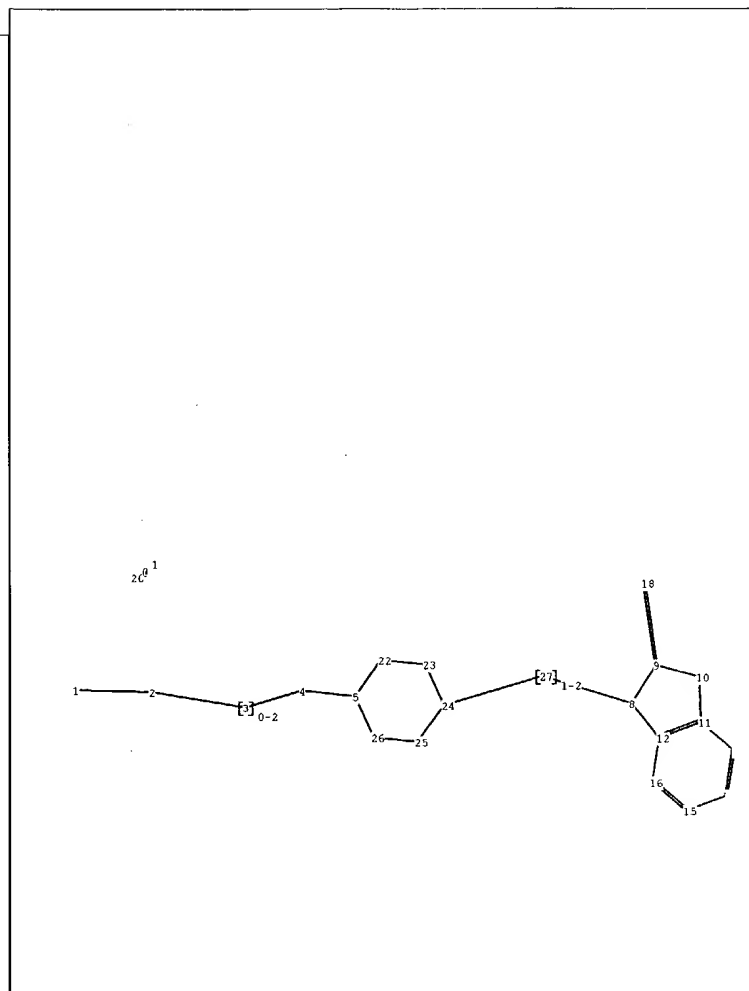
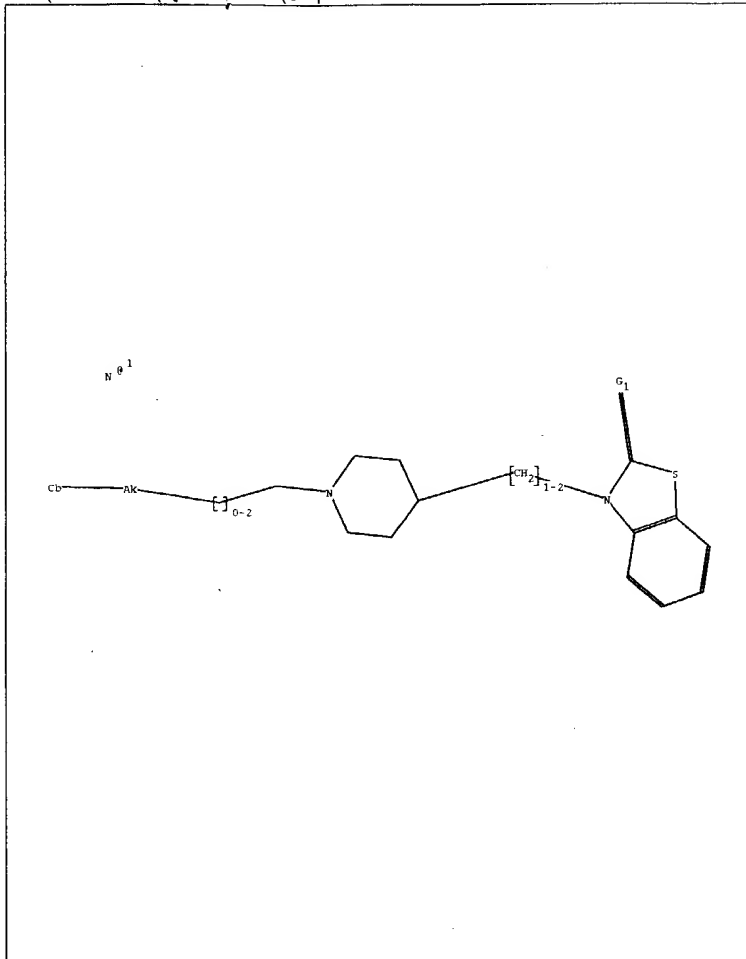
isolated ring systems :

containing 8 :

G1:O,S,[*1]

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 18:CLASS 20:CLASS 22:CLASS



chain nodes :

1 2 3 4 18 20 27

ring nodes :

5 8 9 10 11 12 13 14 15 16 22 23 24 25 26

chain bonds :

1-2 2-3 3-4 4-5 8-27 9-18 24-27

ring bonds :

5-22 5-26 8-12 8-9 9-10 10-11 11-12 11-13 12-16 13-14 14-15 15-16 22-23
23-24 24-25 25-26

exact/norm bonds :

1-2 2-3 4-5 5-22 5-26 8-9 9-18 22-23 23-24 24-25 25-26

exact bonds :

3-4 8-12 8-27 9-10 10-11 24-27

normalized bonds :

11-12 11-13 12-16 13-14 14-15 15-16

isolated ring systems :

containing 8 :

G1:O,S,[*1]

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 18:CLASS 20:CLASS 22:Atom 23:Atom 24:CLASS
25:Atom 26:Atom 27:CLASS

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NEWS 9 SEP 01 INPADOC: New family current-awareness alert (SDI) available
NEWS 10 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
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NEWS 11 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
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NEWS 13 SEP 27 SWETSCAN will no longer be available on STN

NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
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FILE 'HOME' ENTERED AT 15:23:10 ON 20 OCT 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:23:19 ON 20 OCT 2004

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STRUCTURE FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6
 DICTIONARY FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

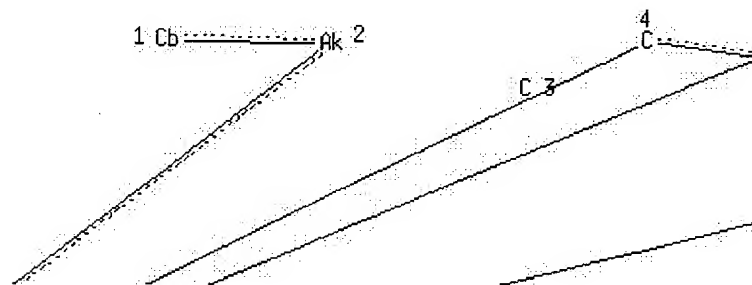
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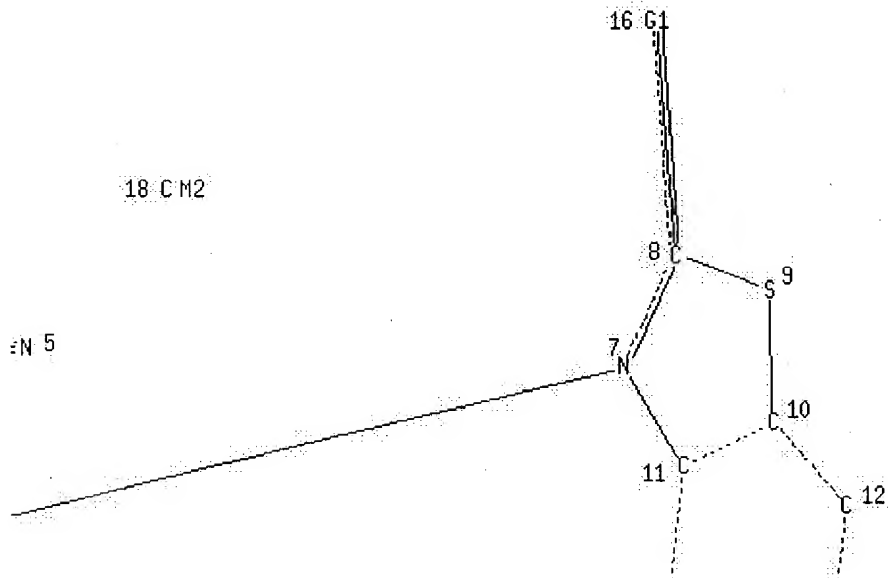
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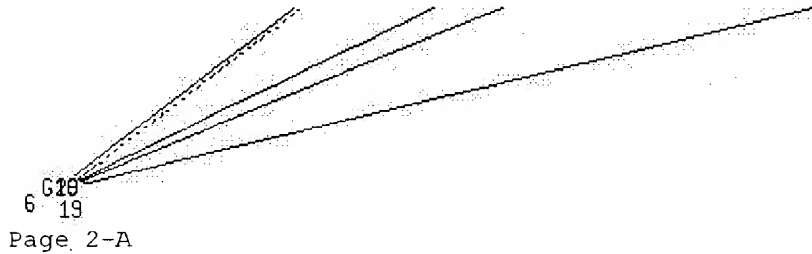
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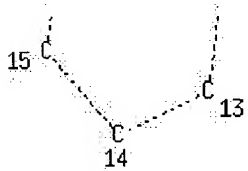
Page 1-A



Page 1-B



Page 2-A



Page 2-B

VAR G1=20/21/17

REP G19=(2-9) 18-5 18-7

REP G20=(0-2) 3-2 3-4

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NSPEC	IS C	AT	1
NSPEC	IS C	AT	2
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NSPEC	IS C	AT	4
NSPEC	IS C	AT	5
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 MLEVEL IS CLASS AT 2 3 4 17 18 20 21
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

=> s 11
 SAMPLE SEARCH INITIATED 15:27:27 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 131 TO ITERATE

100.0% PROCESSED 131 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 1934 TO 3306
 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 15:27:32 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 2447 TO ITERATE

100.0% PROCESSED 2447 ITERATIONS 6 ANSWERS
 SEARCH TIME: 00.00.01

L3 6 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	157.94	158.15

FILE 'HCAPLUS' ENTERED AT 15:27:35 ON 20 OCT 2004
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FILE COVERS 1907 - 20 Oct 2004 VOL 141 ISS 17
 FILE LAST UPDATED: 19 Oct 2004 (20041019/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 5 L3

=> s 14 and rocher, j?/au

75 ROCHER, J?/AU

L5 1 L4 AND ROCHER, J?/AU

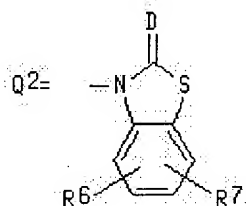
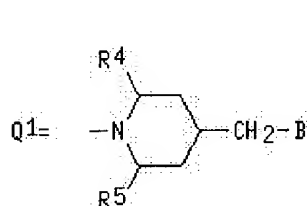
=> d 15, ibib abs fhststr, 1

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citings
References

ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): **Rocher, Jean-Philippe**; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 9923083</u>	A1	19990514	<u>WO 1998-JP4973</u>	19981104
W: CA, CN, KR, US RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
<u>EP 1043319</u>	A1	20001011	<u>EP 1998-951687</u>	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
<u>JP 11217377</u>	A2	19990810	<u>JP 1998-314459</u>	19981105
PRIORITY APPLN. INFO.:			<u>JP 1997-302607</u>	A 19971105
			<u>WO 1998-JP4973</u>	W 19981104
OTHER SOURCE(S):		MARPAT 130:338102		
GI				



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each

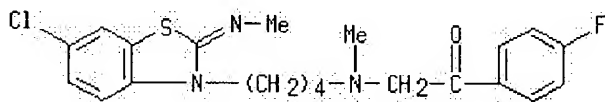
represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups $\text{NR}_3(\text{CH}_2)_p$ and Q1 ; wherein R_3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R_4 and R_5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R_6 and R_7 each represents hydrogen, halogeno, NO_2 , alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxy carbonyl, Ph, (un)substituted NH_2 , alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO , $\text{C}(:\text{NOH})$, $\text{C}(\text{Y})(\text{A})$ (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ -receptors and exhibit small inhibition consts. K_i against σ -1 and/or σ -2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K_2CO_3 followed by NaBH_4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of $[\text{H}_3]$ -di-o-tolylguanidine to σ -receptor (P2 membrane fraction) prepn. from rat liver with K_i value of 7.0 and 3.1 nM, resp., as compared to K_i of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT 224443-03-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-03-2 HCAPLUS

CN Ethanone, 2-[[4-[6-chloro-2-(methylimino)-3(2H)-benzothiazolyl]butyl]methylamino]-1-(4-fluorophenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



#.2 HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 15:23:10 ON 20 OCT 2004)

FILE 'REGISTRY' ENTERED AT 15:23:19 ON 20 OCT 2004

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L2 0 S L1
L3 6 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:27:35 ON 20 OCT 2004

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L6 4 L4 NOT L5

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210 YAMABE, H?/AU

L7 0 L6 AND YAMABE, H?/AU

=> s l6 and chaki, h?/au

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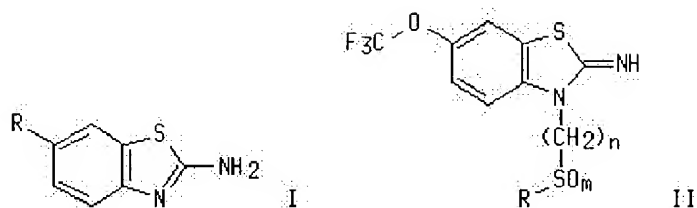
L6 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

References

ACCESSION NUMBER: 1999:420020 HCAPLUS
DOCUMENT NUMBER: 131:144528
TITLE: Riluzole Series. Synthesis and in Vivo "Antiglutamate" Activity of 6-Substituted-2-benzothiazolamines and 3-Substituted-2-imino-benzothiazolines
AUTHOR(S): Jimonet, Patrick; Audiau, Francois; Barreau, Michel; Blanchard, Jean-Charles; Boireau, Alain; Bour, Yvette; Coleno, Marie-Annick; Doble, Adam; Doerflinger, Gilles; Do Huu, Claudine; Donat, Marie-Helene; Duchesne, Jean Marie; Ganil, Pierre; Gueremy, Claude; Honore, Eliane; Just, Bernard; Kerphirique, Roselyne; Gontier, Sylvie; Hubert, Philippe; Laduron, Pierre M.; Le Blevec, Joseph; Meunier, Mireille; Miquet, Jean-Marie; Nemecek, Conception; Pasquet, Martine; Piot, Odile; Pratt, Jeremy; Rataud, Jean; Reibaud, Michel; Stutzmann, Jean-Marie; Mignani, Serge
CORPORATE SOURCE: Centre de Recherche de Vitry-Alfortville, Rhone-Poulenc S.A. Rhone-Poulenc Rorer, Vitry-sur-Seine, F 94403, Fr.
SOURCE: Journal of Medicinal Chemistry (1999), 42(15), 2828-2843
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Two series of analogs of riluzole, a blocker of excitatory amino acid mediated neurotransmission, have been synthesized: monosubstituted 2-benzothiazolamines and 3-substituted derivs. Of all the compds. prepd. in the first series, only 2-benzothiazolamines bearing alkyl, polyfluoroalkyl, or polyfluoroalkoxy substituents in the 6-position showed potent anticonvulsant activity against administration of glutamic acid in rats. The most active compds. displaying in vivo antiglutamate activity were benzothiazolamines I [R = F₃CO (riluzole), F₃CCF₂O, F₃C, F₃CCF₂] with ED₅₀ values between 2.5 and 3.2 mg/kg i.p. Among the second series of variously substituted benzothiazolines, compds. as active as riluzole or up to 3 times more potent were identified in two series: benzothiazolines bearing a β-dialkylaminoethyl moiety and compds. with an alkylthioalkyl chain and their corresponding sulfoxides and sulfones. The most potent derivs. were II [R = Me, m = 0, n = 2; R = Me, m = 1, n = 2] with ED₅₀ = 1.0 and 1.1 mg/kg i.p., resp.. In addn., i.p. administration of some of the best benzothiazolines protected mice from mortality produced by hypobaric hypoxia.

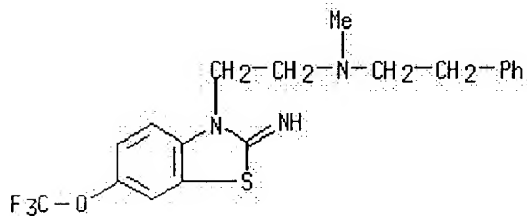
IT **139362-28-0P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of benzothiazolamines and iminobenzothiazolines as anticonvulsant agents)

RN 139362-28-0 HCAPLUS

CN 3(2H)-Benzothiazoleethanamine, 2-imino-N-methyl-N-(2-phenylethyl)-6-(trifluoromethoxy)-, dihydrochloride (9CI) (CA INDEX NAME)



2 HCl

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

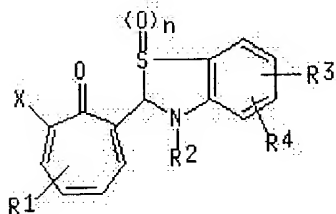
Full Text Citing References

ACCESSION NUMBER: 1993:191730 HCAPLUS

DOCUMENT NUMBER: 118:191730
 TITLE: Preparation of benzothiazolinyltropolones for treatment of ischemia.
 INVENTOR(S): McWhoster, William W.; Ito, Noriie; Ozawa, Kazunori; Kushida, Hiroshi; Nomura, Toshiharu; Kuniyara, Mineo
 PATENT ASSIGNEE(S): Upjohn Co., USA
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04247077	A2	19920903	JP 1991-56252	19910131
CA 2087004	AA	19920301	CA 1991-2087004	19910827
CA 2087004	C	19980421		
EP 546102	A1	19930616	EP 1991-917948	19910827
EP 546102	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 65943	A2	19940829	HU 1993-533	19910827
JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
AT 159251	E	19971115	AT 1991-917948	19910827
ES 2109276	T3	19980116	ES 1991-917948	19910827
NO 9300669	A	19930225	NO 1993-669	19930225
US 5594144	A	19970114	US 1995-442710	19950518
US 5703071	A	19971230	US 1995-443972	19950518
PRIORITY APPLN. INFO.:			JP 1990-229536	19900829
			JP 1991-56252	19910131
			JP 1991-39173	19910208
			WO 1991-US5906	19910827
			US 1993-975924	19930218

OTHER SOURCE(S): MARPAT 118:191730
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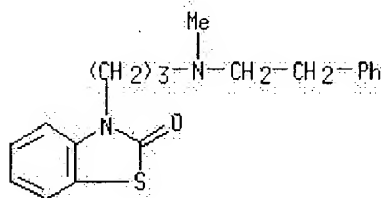
AB The title compds. [I; R1 = H, alkyl, (un)substituted aryl; R2 = H, alkyl, etc.; R3, R4 = H, alkyl, halo, OH, alkoxy, etc.; X = OH, alkoxy, etc.; n = 0, 1, 2] were prepd. E.g., 2-[(2-phenylethyl)amino]thiophenol (prepn. given) was refluxed with 2-methoxy-4-isopropyl-7-formyl-2,4,6-cycloheptatrien-1-one in toluene for 17 H to give I [X = MeO, R1 = 5'-iso-Pr, R2 = PhCH2CH2, R3 = R4 = H, n = 0]. At 0.1 mg/Kg i.p. this showed 50% effectiveness in counteracting brain ischemic rats in a learning study using rats.

IT 142224-30-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for benzothiazolinyltropolones for

treatment of ischemia)

RN 142224-30-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-[methyl(2-phenylethyl)amino]propyl]- (9CI)
(CA INDEX NAME)

L6 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical References
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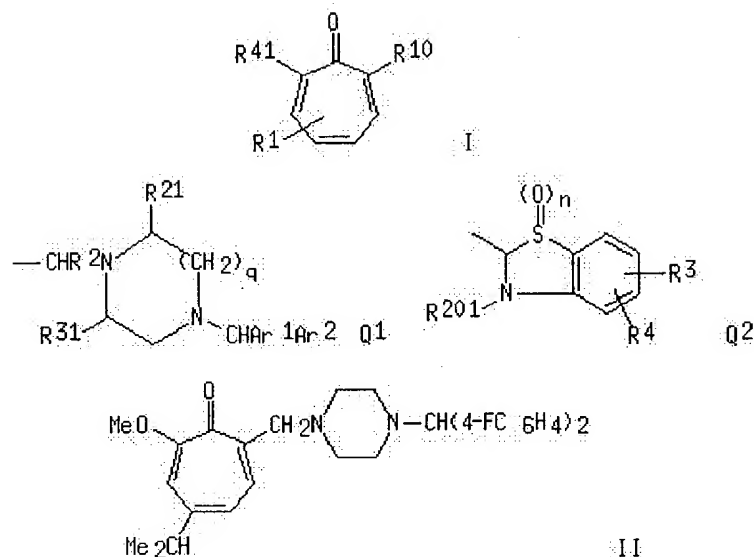
ACCESSION NUMBER: 1992:531223 HCAPLUS
DOCUMENT NUMBER: 117:131223
TITLE: Preparation of heterocyclyltropolones as ischemia inhibitors
INVENTOR(S): Ito, Noriie; Kuniyara, Mineo; Kushida, Hiroshi; McWhorter, William W.; Nomura, Syunji; Ozawa, Kazunori; Taniguchi, Mikeo; Tsuzuki, Tazuo
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9204338	A1	19920319	WO 1991-US5906	19910827
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MC, MG, MN, MW, NO, PL, RO, SD, SU, US				
RW: AT, BE, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN				
JP 04120069	A2	19920421	JP 1990-229536	19900829
AU 9187203	A1	19920330	AU 1991-87203	19910827
AU 651629	B2	19940728		
EP 546102	A1	19930616	EP 1991-917948	19910827
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JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
NO 9300669	A	19930225	NO 1993-669	19930225

PRIORITY APPLN. INFO.:

JP 1990-229536	19900829
JP 1991-56252	19910131
JP 1991-39173	19910208
WO 1991-US5906	19910827

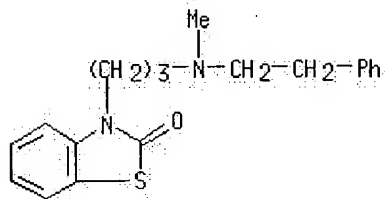
OTHER SOURCE(S): MARPAT 117:131223
GI



AB Title compds. I [R10 = Q1, Q2; R1, R2 = H, C1-5 alkyl, (substituted) aryl, (substituted) heterocyclyl; R3, R4 = H, (substituted) C1-5 alkyl, C7-20 aralkyl, C7-20 aralkyl contg. O, S, or N atoms; halo, OH, C1-5 alkoxy, cyano, etc.; R41 = OR3, OR6, NR7R8, etc.; R6 = H, (substituted) C1-5 alkyl, etc.; R7, R8 = H, (substituted) C1-5 alkyl, C7-20 aralkyl which may contain O, S, or N atoms; NR7R8 = 5-7 membered ring which may contain addnl. O or N atoms; R21, R31 = H, C1-3 alkyl; R201 = H, C1-5 alkyl, C2-20 aralkyl, C6-10 arylsulfonyl, C6-10 arylsulfonyl contg. O, S, or N atoms; Ar1, Ar2 = (substituted) aryl; n = 0-2; q = 1-2], were prepd. Thus, a soln. of 7-chloromethyl-4-isopropyl-2-methoxy-4-isopropyl-2,4,6-cycloheptatrien-1-one (prepn. given), 1-(4,4'-difluorobenzhydryl)piperazine, and Et₃N in CHCl₃ was refluxed for 20 h to give title compd. II. II had minimal ED of <5 mg/kg i.v. in a ischemic heart/reperfusion test in rats.

IT **142224-30-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for ischemia inhibitors)
 RN 142224-30-4 HCAPLUS
 CN 2(3H)-Benzothiazolone, 3-[3-[methyl(2-phenylethyl)amino]propyl]- (9CI)
 (CA INDEX NAME)



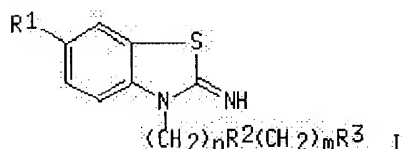
L6 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citations
 References

ACCESSION NUMBER: 1992:128911 HCAPLUS
 DOCUMENT NUMBER: 116:128911
 TITLE: Benzothiazoline derivatives, process for their preparation, and drugs containing them
 INVENTOR(S): Gueremy, Claude; Jimonet, Patrick; Mignani, Serge
 PATENT ASSIGNEE(S): Rhone-Poulenc Rorer SA, Fr.
 SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9118892	A1	19911212	WO 1991-FR437	19910531
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
FR 2663029	A1	19911213	FR 1990-7068	19900607
FR 2663029	B1	19920731		
CA 2080005	AA	19911208	CA 1991-2080005	19910531
EP 532602	A1	19930324	EP 1991-910896	19910531
EP 532602	B1	19940803		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05507918	T2	19931111	JP 1991-510727	19910531
ES 2057901	T3	19941016	ES 1991-910896	19910531
US 5340824	A	19940823	US 1992-938153	19921202
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OTHER SOURCE(S):		MARPAT 116:128911		
GI				



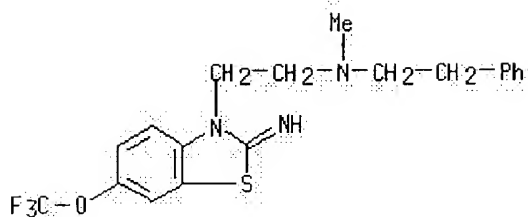
AB Benzothiazolines I [R1 = polyfluoroalkoxy; R2 = S, alkylimino, SO, SO₂; R3 = Ph, Bz, NR₄R₅, 1-(phenylalkyl)-4-piperidinyl; R4 = alkyl; R5 = phenylalkyl; n = 1-3; m = 0-3] and salts are prepd. as drugs for treating convulsions, schizophrenia, sleep disorders, cerebral ischemic phenomena, glutamate-related neurol. disorders, Alzheimer's disease (no data). For example, thioetherification of PhCH₂NMeCH₂CH₂SH with 2-[2-(trifluoroacetylimino)-6-(trifluoromethoxy)-3-benzothiazolinyl]ethyl p-toluenesulfonate (prepd. in 3 steps) and subsequent salification gave I (R1 = CF₃O, R2 = S, R3 = NMeCH₂Ph, n = m = 2) as the dioxalate salt. Nine syntheses and 3 formulations are described.

IT 139362-28-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as neurol. drug)

RN 139362-28-0 HCAPLUS

CN 3(2H)-Benzothiazoleethanamine, 2-imino-N-methyl-N-(2-phenylethyl)-6-(trifluoromethoxy)-, dihydrochloride (9CI) (CA INDEX NAME)



2 HCl

=> file caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

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CA SUBSCRIBER PRICE

-3.50

-3.50

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L6 4 S L4 NOT L5

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FULL ESTIMATED COST

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CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6

DICTIONARY FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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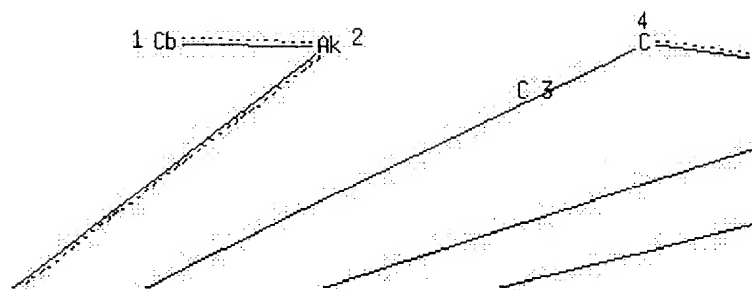
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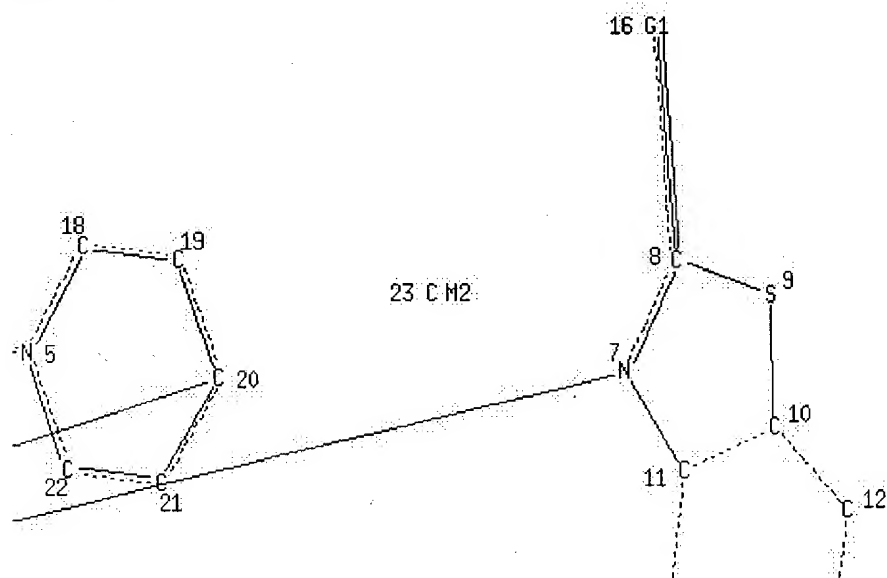
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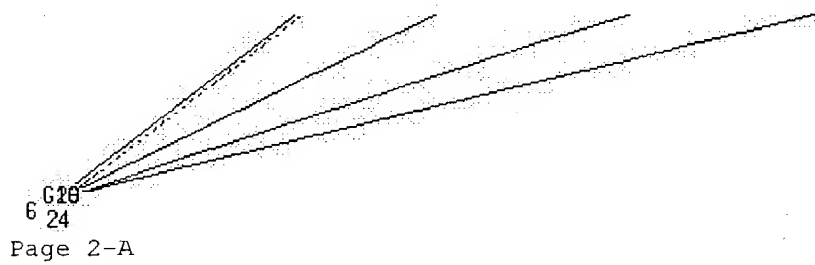
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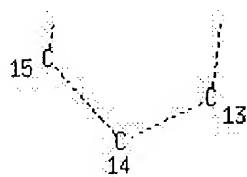
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Page 1-B



Page 2-A



Page 2-B

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REP G20=(0-2) 3-2 3-4

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NUMBER OF NODES IS 26

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3 ANSWERS

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FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 22 TO 418

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THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

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FULL ESTIMATED COST	156.26	343.35
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.50

FILE 'HCAPLUS' ENTERED AT 15:30:52 ON 20 OCT 2004
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FILE COVERS 1907 - 20 Oct 2004 VOL 141 ISS 17
 FILE LAST UPDATED: 19 Oct 2004 (20041019/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l15

L16 1 L15

=> d l16, ibib abs fhitstr, 1

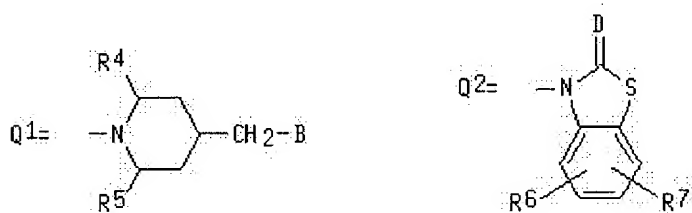
L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical Abstracts
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ACCESSION NUMBER: 1999:311193 HCAPLUS
 DOCUMENT NUMBER: 130:338102
 TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
 INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
 SOURCE: PCT Int. Appl., 95 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607	A 19971105
			WO 1998-JP4973	W 19981104
OTHER SOURCE(S):	MARPAT 130:338102			
GI				



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxy carbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ -receptors and exhibit small inhibition consts. K_i against σ -1 and/or σ -2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K_2CO_3 followed by $NaBH_4$ redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of $[H_3]$ -di-o-tolylguanidine to σ -receptor (P2 membrane fraction) prepn. from rat liver with K_i value of 7.0 and 3.1 nM, resp., as compared to K_i of 29 nM for

haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

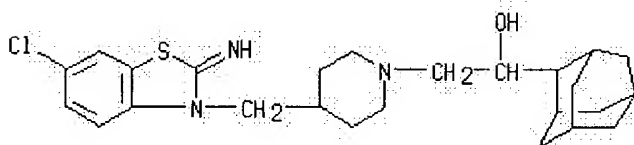
IT 224442-60-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224442-60-8 HCAPLUS

CN 1-Piperidineethanol, 4-[(6-chloro-2-imino-3(2H)-benzothiazolyl)methyl]- α -tricyclo[3.3.1.1^{3,7}]dec-2-yl-, dihydrochloride (9CI) (CA INDEX NAME)



2 HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
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FULL ESTIMATED COST

7.12	350.47
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE

-0.70	-4.20
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FILE 'CAOLD' ENTERED AT 15:31:06 ON 20 OCT 2004

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter [HELP FIRST](#) for more information.

=> d his

(FILE 'HOME' ENTERED AT 15:23:10 ON 20 OCT 2004)

FILE 'REGISTRY' ENTERED AT 15:23:19 ON 20 OCT 2004

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 6 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:27:35 ON 20 OCT 2004

L4 5 S L3
L5 1 S L4 AND ROCHER, J?/AU
L6 4 S L4 NOT L5
L7 0 S L6 AND YAMABE, H?/AU
L8 0 S L6 AND CHAKI, H?/AU
L9 0 S L6 AND SAITO, K?/AU
L10 0 S L6 AND ABE, M?/AU
L11 0 S L6 AND OKUYAMA, M?/AU

FILE 'CAOLD' ENTERED AT 15:28:46 ON 20 OCT 2004

L12 0 S L3

FILE 'REGISTRY' ENTERED AT 15:28:52 ON 20 OCT 2004

L13 STRUCTURE UPLOADED
L14 3 S L13
L15 89 S L13 FULL

FILE 'HCAPLUS' ENTERED AT 15:30:52 ON 20 OCT 2004

L16 1 S L15

FILE 'CAOLD' ENTERED AT 15:31:06 ON 20 OCT 2004

=> s l15

L17 0 L15

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